First Principles Approach to Functional Aqueous Semiconductor Interfaces

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Understanding structure-property relationships for materials in such applications as energy storage and photocatalysis pose significant challenges for theory. In this talk, I will briefly describe first principles approaches to calculate the properties of aqueous semiconductor interfaces. Specifically, I will address: (1) interface structure; (2) the alignment of semiconductor band edges to redox levels in water; and (3) examples of chemical functionality. The exemplary materials will largely be GaN, ZnO and alloys, motivated by observations of visible light absorption in alloys and efficient photocatalytic water splitting by the Domen group.

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